CONTENTS

Special Issue: Theoretical Chemistry 1989 – Proceedings of the XVIIIth International Congress of the Theoretical Chemists of Latin Expression held at La Plata, Argentina, 23–28 September 1989

Editorial ix

A new methodology in quantum chemistry: use of partially orthogonalized orbitals
E. Gianinetti and I. Vandoni (Milan, Italy) 1
Kohn–Sham theory and the representability problem
E.V. Ludeña and V. Mujica (Caracas, Venezuela) 9
Chemical reactivity in density functional theory: the *N*-differentiability problem
J.L. Gázquez, M. Galván and A. Vela (Mexico, Mexico) 29
Density matrix of fermionic systems from coherent states via functional integrals
H. Grinberg (Buenos Aires, Argentina) and J.Marañon (La Plata, Argentina) 39
Application of the exponential propagation matrix method to the numerical solution of the Schrödinger equation
C.G. Díaz (Mar del Plata, Argentina), F.M. Fernández and E.A. Castro (La Plata, Argentina) 45
Polynomial expressions for Rydberg–Klein–Rees curves of diatomic covalent molecules
E. Daza and J.L. Villaveces (Bogotá, Colombia), G. Arteca (Saskatoon, Sask., Canada), F. Fernández and E. Castro (La Plata, Argentina) 49
Generator coordinate Gaussian expanded natural orbitals
H.F.M. Da Costa, A.B.F. Da Silva and M. Trsic (São Carlos, Brazil), A.M. Simas (Recife, Brazil) and A.J.A. Aquino (São Paulo, Brazil) 63
Sequence transformations for the efficient evaluation of infinite series representations of some molecular integrals with exponentially decaying basis functions
E. O. Steinborn and E.J. Weniger (Regensburg, F.R.G.) 71
Application of the distance between subspaces to the evaluation of wavefunction quality
J.M. Garcia De La Vega and B. Miguel (Madrid, Spain) 79
Virial-type relations for arbitrary subsystems of particles belonging to a molecular system
M. García-Sucre (Caracas, Venezuela) 85
Statistical population analysis of spin distributions for molecular systems
H.F. Reale and R.C. Bochicchio (Buenos Aires, Argentina) 93
On the electronic distribution for extended systems. Part II. Condensation and long-range-order correlations for fermion pairs
R.C. Bochicchio (Buenos Aires, Argentina) 99
Localization method for semiempirical molecular orbitals based on the Boys–Foster criterion
C.N. Cavasotto, C.G. Giribet and R.H. Contreras (Buenos Aires, Argentina) 107
The properties of polycyclic hydrocarbons: on the theory of incremental methods
J.A.N.F. Gomes (Porto, Portugal) 111
Effective nuclear charges through the fitting of atomic polarizabilities with density functionals
M.C. Donnamaría (Trieste, Italy), R.E. Cachau and E.A. Castro (La Plata, Argentina) 121
Use of perturbed first-order density matrices in multi-reference configuration interaction expansions
G. Berthier (Paris, France), A. Daoudi (Fès-Atlas, Morocco), G. Del Re (Naples, Italy) and J.P. Flament (Palaiseau, France) 133
Electronic structure of metal monocarbonyls
A. Daoudi (Palaiseau, France, and Fès-Atlas, Morocco), M. Suard (Palaiseau, France, and Montrouge, France) and G. Berthier (Paris, France) 139

CONTENTS

Special Issue: Theoretical Chemistry 1989 – Proceedings of the XVIIIth International Congress of the Theoretical Chemists of Latin Expression held at La Plata, Argentina, 23–28 September 1989

Editorial ix

A new methodology in quantum chemistry: use of partially orthogonalized orbitals
E. Gianinetti and I. Vandoni (Milan, Italy) 1
Kohn–Sham theory and the representability problem
E.V. Ludeña and V. Mujica (Caracas, Venezuela) 9
Chemical reactivity in density functional theory: the *N*-differentiability problem
J.L. Gázquez, M. Galván and A. Vela (Mexico, Mexico) 29
Density matrix of fermionic systems from coherent states via functional integrals
H. Grinberg (Buenos Aires, Argentina) and J.Marañon (La Plata, Argentina) 39
Application of the exponential propagation matrix method to the numerical solution of the Schrödinger equation
C.G. Díaz (Mar del Plata, Argentina), F.M. Fernández and E.A. Castro (La Plata, Argentina) 45
Polynomial expressions for Rydberg–Klein–Rees curves of diatomic covalent molecules
E. Daza and J.L. Villaveces (Bogotá, Colombia), G. Arteca (Saskatoon, Sask., Canada), F. Fernández and E. Castro (La Plata, Argentina) 49
Generator coordinate Gaussian expanded natural orbitals
H.F.M. Da Costa, A.B.F. Da Silva and M. Trsic (São Carlos, Brazil), A.M. Simas (Recife, Brazil) and A.J.A. Aquino (São Paulo, Brazil) 63
Sequence transformations for the efficient evaluation of infinite series representations of some molecular integrals with exponentially decaying basis functions
E. O. Steinborn and E.J. Weniger (Regensburg, F.R.G.) 71
Application of the distance between subspaces to the evaluation of wavefunction quality
J.M. Garcia De La Vega and B. Miguel (Madrid, Spain) 79
Virial-type relations for arbitrary subsystems of particles belonging to a molecular system
M. García-Sucre (Caracas, Venezuela) 85
Statistical population analysis of spin distributions for molecular systems
H.F. Reale and R.C. Bochicchio (Buenos Aires, Argentina) 93
On the electronic distribution for extended systems. Part II. Condensation and long-range-order correlations for fermion pairs
R.C. Bochicchio (Buenos Aires, Argentina) 99
Localization method for semiempirical molecular orbitals based on the Boys–Foster criterion
C.N. Cavasotto, C.G. Giribet and R.H. Contreras (Buenos Aires, Argentina) 107
The properties of polycyclic hydrocarbons: on the theory of incremental methods
J.A.N.F. Gomes (Porto, Portugal) 111
Effective nuclear charges through the fitting of atomic polarizabilities with density functionals
M.C. Donnamaría (Trieste, Italy), R.E. Cachau and E.A. Castro (La Plata, Argentina) 121
Use of perturbed first-order density matrices in multi-reference configuration interaction expansions
G. Berthier (Paris, France), A. Daoudi (Fès-Atlas, Morocco), G. Del Re (Naples, Italy) and J.P. Flament (Palaiseau, France) 133
Electronic structure of metal monocarbonyls
A. Daoudi (Palaiseau, France, and Fès-Atlas, Morocco), M. Suard (Palaiseau, France, and Montrouge, France) and G. Berthier (Paris, France) 139

A theoretical study of solvent effects on the relative thermodynamic stabilities of the allyl$^+$/F^- and allyl$^-$/Li^+ ion pairs in polar media
R.R. Contreras, L. Padilla and J.S. Gomez–Jeria (Casilla, Chile) and A.J. Aizman (Valparaiso, Chile) 147
Cationic structures of acetamidoxime: theoretical analysis of H^+ and Li^+ complexes
G. La Manna (Palermo, Italy) and M. Cignitti (Rome, Italy) 161
Quantum topological description of the charge density of the ON–NO_2 and ON–NSO molecules
O.G. Stradella, S.A. Maluendes and E.A. Castro and A.H. Jubert (La Plata, Argentina) 169
Quantum chemical analysis of the orientational lone-pair effect on spin–spin coupling constants
R.H. Contreras, C.G. Giribet, M.C. Ruiz de Azúa and C.N. Cavasotto (Buenos Aires, Argentina), G.A. Aucar (Corrientes, Argentina) and L.B. Krivdin (Irkutsk, U.S.S.R.) 175
Molecular orbital theory: diagramatic representation of the contribution of the magnetic anisotropy effect on the magnetic shielding constant
M.B. Ferraro and R.H. Contreras (Buenos Aires, Argentina) 187
Analysis of the diamagnetic spin–orbital contribution to indirect nuclear spin–spin coupling constants
J.E. Pérez and F.S. Ortiz (Córdoba, Argentina), R.H. Contreras, C.G. Giribet and M.C. Ruiz de Azúa (Buenos Aires, Argentina) 193
The use of the SPPA method for the semi-empirical analysis of indirect spin couplings in Si-containing compounds
R. Righini, C.G. Giribet, M.C. Ruiz de Azua and R.H. Contreras (Buenos Aires, Argentina) ... 199
Large spin–dipolar long-range F–F coupling constants in conjugative compounds: their study using propagators
N.M. Peruchena and G.A. Aucar (Corrientes, Argentina) and R.H. Contreras (Buenos Aires, Argentina) 205
Theoretical and experimental study of the orientational oxygen lone-pair effect on $^1J(^{13}C–^1H)$ in methoxy- and methylene-dioxybenzene compounds
R.R. Biekofsky and A.B. Pomilio and R.H. Contreras (Buenos Aires, Argentina) 211
Photoionization in phase space
G.P. Arrighini, C. Guidotti and N. Durante (Pisa, Italy) 221
A time-dependent approach to the intramolecular vibrational relaxation mechanism. An application to the $Ar\cdots Cl_2(B)$ complex
S. Serna, P. Villarreal, S. Miret-Artés, J. Campos-Martinez and G. Delgado-Barrio (Madrid, Spain) 227
Energetics of small $BC\cdots X_n$ van der Waals clusters. Application to $I_2\cdots Ne_n$ (n= 1–3)
A. García-Vela, P. Villarreal and G. Delgado-Barrio (Madrid, Spain) 237
Doubly excited states of B_2, B_2^+, B_2^{2+} and B_2^-
P.J. Bruna and J.S. Wright (Ottawa, Ont., Canada) 243
Oscillator strengths for XeII transitions
D. Iriarte and H.O. Di Rocco (Tandil, Argentina), M. Raineri, J. Reyna Almandos and M. Gallardo (La Plata, Argentina) 253
Theoretical transition probabilities and lifetimes for the BeH^+ ($A^1\Sigma^+ - X^1\Sigma^+$) band system
F.B.C. Machado (São José dos Campos, Brazil) and F.R. Ornellas (São Paulo, Brazil) 259
On the conjugation in macrocycles: the electronic structure and spectrum of hemiporphyrazine
M. Bossa, I. Grella, P. Nota and E. Cervone (Rome, Italy) 267
Potential-energy hypersurface for large-amplitude coordinates in dimethylamine
Y.G. Smeyers, M. Fernandez and V. Botella (Madrid, Spain) 273
On the rotational isomerism of one rotor molecules. A comparative study of the HSSH and HXNX (X=O, S) series of molecules
G.I. Cárdenas-Jirón, C. Cárdenas-Lailhacar and A. Toro-Labbé (Santiago, Chile) 279

Ab initio study of internal rotation in 2-pyridincarboxaldehyde
Y.G. Smeyers and A. Hernández-Laguna (Madrid, Spain), M.J. Martìn-Delgado, M.J. Macedo and M.I. Suero (Badajoz, Spain) 291
SCF–LCAO–MO study of the internal rotation and tilt angle in propyl fluoride
Y.G. Smeyers, A. Hernández-Laguna, M.J. Moreno-Recio and P. Sanchez-Gómez (Madrid, Spain) 299
Ab initio study of the vibrational properties of perfluoroacetaldehyde
E. Ottavianelli, S. Maluendes, E. Castro and A. Jubert (La Plata, Argentina) 305
Non-covalent interactions in bimolecular up to mesoscopic systems
J. Tomasi, G. Alagona, R. Bonaccorsi and C. Ghio (Pisa, Italy) and R. Cammi (Parma, Italy) 311
Ab initio calculation of gas-phase methyl radical formation over $Mg^{2+}O^{2-}$ and $Li^{+}O^{-}$ adsorption model sites
J. Rodríguez, Y. Aray and F. Ruette (Caracas, Venezuela) 325
H_2 on MoS_2: a molecular orbital study
R. Pis Diez and A.H. Jubert (La Plata, Argentina) 329
Activation of the hydrogen bond by transition metals
E. Poulain, F. Colmenares, S. Castillo and O. Novaro (México, Mexico) 337
Theoretical study of underpotential deposition of foreign metal atoms on Pt(111) single-crystal cluster surfaces. Part 1. The stability of the different metal underpotential-deposition layer structures as a function of surface coverage and applied electric potential
M.B. López, G.L. Estiú, E.A. Castro and A.J. Arvía (La Plata, Argentina) 353
Theoretical study of underpotential deposition of foreign metal atoms on Pt(111) single-crystal cluster surfaces. Part 2. The influence of metal underpotential deposition layer structures on the decomposition of co-adsorbed water
M.B. López, G.L. Estiú, E.A. Castro and A.J. Arvia (La Plata, Argentina) 365
A quantum chemistry approach to the electro-oxidation of CO adsorbed on Rh(111) cluster surfaces
P. Paredes Olivera, G.L. Estiú, E.A. Castro and A.J. Arvía (La Plata, Argentina) 379
Theoretical study of the influence of the applied electric potential and the co-adsorption of water on the vibrational properties of CO adsorbed on Rh(111)
P. Paredes Olivera, G.L. Estiú, E.A. Castro and A.J. Arvia (La Plata, Argentina) 393
Theoretical studies of hydrogen-bonded complexes using semiempirical methods
E.L. Coitiño, K. Irving, J. Rama, A. Iglesias, M. Paulino and O.N. Ventura (Montevideo, Uruguay) 405
Comparison of semiempirical and BSSE corrected Møller–Plesset ab initio calculations on the direct addition of water to formaldehyde
O.N. Ventura, E.L. Coitiño, K. Irving and A. Iglesias (Montevideo, Uruguay) and A. Lledós (Catalonia, Spain) 427
MNDO and AM1 estimation of the electrostatic, induction and dispersion contributions to the solvation energy by a continuum model
E.Sanchez Marcos, M.J. Capitán, M. Galán and R.R. Pappalardo (Seville, Spain) 442
Structure–activity relationships for histamine H_2-antagonists
F.M.L.G. Stamato, M.A. Perez and E. Longo (São Carlos, Brazil) 447
GAMYR: a generalized version of AMYR for the study of biomolecules
E.A. Bidacovich (Avellaneda, Argentina), S.G. Kalko and R.E. Cachau (La Plata, Argentina) 455
Molecular modelling of glutathione: a comparison with crystallographic data
M.P. De Blumenfeld, N. Hikichi, M. Hansz and O. N. Ventura (Montevideo, Uruguay) 469

Author index 477

Subject index 479